ON THE ORIGIN OF EXTRA PEAKS IN THE DIELECTRIC FUNCTION OF $Si_{1-x-y}Ge_xC_y$ ALLOYS GROWN PSEUDOMORPHICALLY ON SI (001)

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1. INTRODUCTION

Several spectroscopic ellipsometry studies of $Si_{1-y}C_y$ alloys (y <2%) grown pseudomorphically on Si have recently appeared in the literature. One of these (by Lee, Floro, Strane, Lee, Jones, Mayer, and Picraux) reports additional peaks below the E_1 peak, which is usually considered to be the lowest direct band gap for silicon-type materials. We present simulated spectra of such sample structures and show that the additional peaks are due to interference effects (when the incident light is reflected at the epilayer-substrate interface) and not due to intrinsic properties of the material. We compare these simulated spectra with experimental data and also present an empirical model for the dielectri function of $Si_{1-y}C_y$ alloys on Si.

2. PROBLEM

The band structure and critical-point energies of supersaturated $Si_{1-y}C_y$ alloys[1, 2] (y <0.02) have recently been the origin of some controversy in the literature. Osten *et al.*[2, 3] and Zollner *et al.*[4, 5] have found using electroreflectance and spectroscopic ellipsometry that the E_1 energies of such alloys increase linearly with increasing C content, as expected from a simple virtual-crystal alloy picture. Using established deformation potentials for Si and assuming ideal pseudomorphic growth, it is possible to explain the observed E_1 energies if the shifts due to biaxial strain and composition are properly taken into account.[4]

Demkov and Sankey[6] have argued, on the other hand, that the band gaps of free-standing (unstrained) $Si_{1-y}C_y$ alloys should decrease with increasing carbon content. Therefore, for *strained* pseudomorphic alloys, the lower of the two strain-split E_1 energies (which is not expected to be observed when probing with light at or near normal incidence) should decrease even more. Additional weak structures in the dielectric functions of $Si_{1-y}C_y$ and $Si_{1-x-y}Ge_xC_y$ alloys (fabricated using C implantation followed by solid phase epitaxial growth) at 2.7 eV and 3.0 eV (below the E_1 energy near 3.4 eV) were indeed reported by Lee *et al.*[7] These structures were interpreted as previously unidentified optical transitions in

the material. In this work, we argue that the new structures are actually interference fringes originating from the reflection of light at the alloy-substrate interface. We present simple model calculations for this effect and compare our results with experimental data obtained with spectroscopic ellipsometry.

3. SOLUTION

The dielectric response of a stratified planar structure (ambient-epilayer-substrate) can be calculcated if the dielectric functions of all materials as well as the thickness of the epitaxial layer are known.[8] The dielectric function $\epsilon(E)$ can be described either in tabulated form (i.e., values of ϵ for a given set of energies E or wavelengths λ) or in parametrized form. A parameter model for Si is more appropriate for our purposes, since it can be transferred to $Si_{1-y}C_y$ alloys by changing some of the parameters as described below.

However, these parameter models are not unproblematic: As described by Kim *et al*,[9] a model optimized to fit the dielectric function will usually not describe the derivatives very well and vice versa. Therefore, a model should simultaneously be fit to $\epsilon(E)$ and its first three derivatives. This was done for GaAs,[9] but we are not aware of similar work for Si. Therefore, we had to use a parameter set obtained by fitting ϵ, which does not describe $d^2\epsilon/dE^2$ very well.

We have used the parameters of Adachi[10] to model the dielectric function ϵ of Si, since it describes the second derivative $d^2\epsilon/dE^2$ (calculated using the Savitzky-Golay method by fitting a 5th order polynomial to 13 data points) somewhat better than the similar model of Forouhi.[11] After most of this work was completed we became aware of a more recent model for Si,[12] where the parameters were optimized to fit the dielectric function as well as its first derivative (determined using thermoreflectance). Nevertheless, this model does not fit the second derivative very well. We repeated all of our calculations with this new model, but did not see any significant changes in the figures. We also note that the dielectric function (even in the absence of an oxide overlayer) depends somewhat on the sample parameters (for example on impurity and doping concentration). However, the failure of Adachi's model[10] to describe the second derivatives cannot be explained with this argument, since the discrepancies are much larger than the effect of doping on the second derivative.

For the dielectric function of $Si_{1-y}C_y$ alloys (more precisely: for the **ordinary** dielectric function describing light travelling along the growth direction) we use the Si parameters of Adachi[10] with the following modifications: The E_1 energy is increased[13] by 0.05 eV per percent C. The broadening of the E_1 critical point is increased by 50% compared to Si in order to describe the lower amplitude of the derivative observed in the experimental spectra. All other parameters (including the E_0' and E_2 energies) were left unchanged. We assumed a thickness of the epilayer of 200 nm.

For completeness (although this is not relevant for the issue of the extra peaks), we also mention briefly how to model the dielectric function of $Si_{1-y}C_y$ alloys for a beam of

light travelling in the plane (perpendicular to the growth direcction). In this case, we have to distinguish between two cases, since the crystal is under biaxial strain[4] and therefore uniaxial, with the optical axis being identical to the growth direction. (i) The electric field vector $\vec{E}$ is perpendicular to the growth direction (ordinary beam). (ii) $\vec{E}$ is parallel to the growth direction (extraordinary beam). In the ordinary case, ϵ is the same as for a beam propagating along the growth direction. In the extraordinary case, theory predicts[4] (this has not been observerd in $Si_{1-y}C_y$ alloys, only in Si[14]) that the component of E_1 coupling to the beam should approximately be independent of y (since the strain shifts cancel the shifts due to alloy composition). Therefore, it is suggested that the Si parameters of Adachi should be used to model the extraordinary refractive index of $Si_{1-x}C_x$. Probably the broadening parameter for E_1 should be increased by about 50%, just like in the ordinary case.

We note that when modeling the optical properties of $Si/Si_{1-y}C_y$ heterostructures, the Adachi parameters should be used for both Si and (slightly modified as described above) for the epilayer. Using the measured dielectric function for Si together with the modified Adachi parameters for the alloy layer will lead to inconsistencies, since the gaps in the model are somewhat different from the measured critical-point energies.

4. DISCUSSION

The calculated pseudodielectric function for a $Si_{1-y}C_y$ film (grown pseudomorphically on Si) with 1.5% C and 200 nm thickness is shown in Fig. 1. Oscillatory features due to the reflection of light at the epilayer-substrate interface are visible below, but not above E_1,

Figure 1: Dielectric function of $Si_{1-y}C_y$ and $y = 1.5\%$

since the penetration depth in Si changes drastically from about 12 μm at 1.5 eV to 6.9 nm at 4 eV, see Ref. [15]. These oscillations are much more pronounced, if the second derivative $d^2\epsilon/dE^2$ is plotted in the E_1 region, see Fig. 2 (a). For comparison, we also show experimental data of a sample with the same parameters, see Fig. 2 (b). The symbols

Figure 2: Second derivative of the dielectric function of $Si_{1-y}C_y$ and ($y = 1.5\%$). (a) modeled function, (b) measured data and fit

indicate the experimental data, i.e., the real (•) and imaginary part (△) of ϵ, and the lines show a fit with an analytical line shape.[4] Note that the difference between the experimental data and the analytical line shape oscillates much more below E_1 than above. While we do not intend to make a one-to-one comparison of all features in the simulated and measured spectra, there is a striking similarity of the oscillations in both parts of the figure. The peak positions in the measured and modelled spectra differ by about 150 meV, since Adachi's parameters do not quite accurately describe $d^2\epsilon/dE^2$ for Si, as explained above.

5. CONCLUSION

In conclusion, we have shown that the weak structures below 3.4 eV in the pseudodielectric function of $Si_{1-y}C_y$ alloys are due to the reflection of light at the epilayer-substrate interface. For an ideal stratified structure, it is possible in principle to remove such interference fringes using a commercial software package,[16] but in practice this may be difficult due to sample imperfections. It has also been argued[17] that the numerical removal of overlayer/substrate effects may increase the noise in the spectra and therefore may make the lineshape analysis more difficult. We also mention that the optical contrast is much bigger

between $Si_{1-x-y}Ge_xC_y$ and Si than for $Si_{1-y}C_y$ and Si.[18] Therefore, the observed fringes are stronger in the former system than in the latter, which was observed experimentally.[7]

6. ACKNOWLEDGEMENT

This work was supported in part by the National Science Foundation (grant no. DMR-9413492) and by Ames Laboratory, which is operated for the U.S. Department of Energy by Iowa State University under Contract No. W-7405-Eng-82. Part of this work was supported by the Director for Energy Research, Office of Basic Energy Sciences. A. A. A. was supported by the Ames Laboratory Summer Trainee Program. The sample used in this study was grown by S. S. Iyer, K. Eberl, and A. P. Powell at the IBM T. J. Watson Research Center as described elsewhere.[1]

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